

Supplementary Materials for

**The record low thermal conductivity of monolayer Cuprous Iodide (CuI) with
direct wide bandgap**

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Note S1: High temperature stability

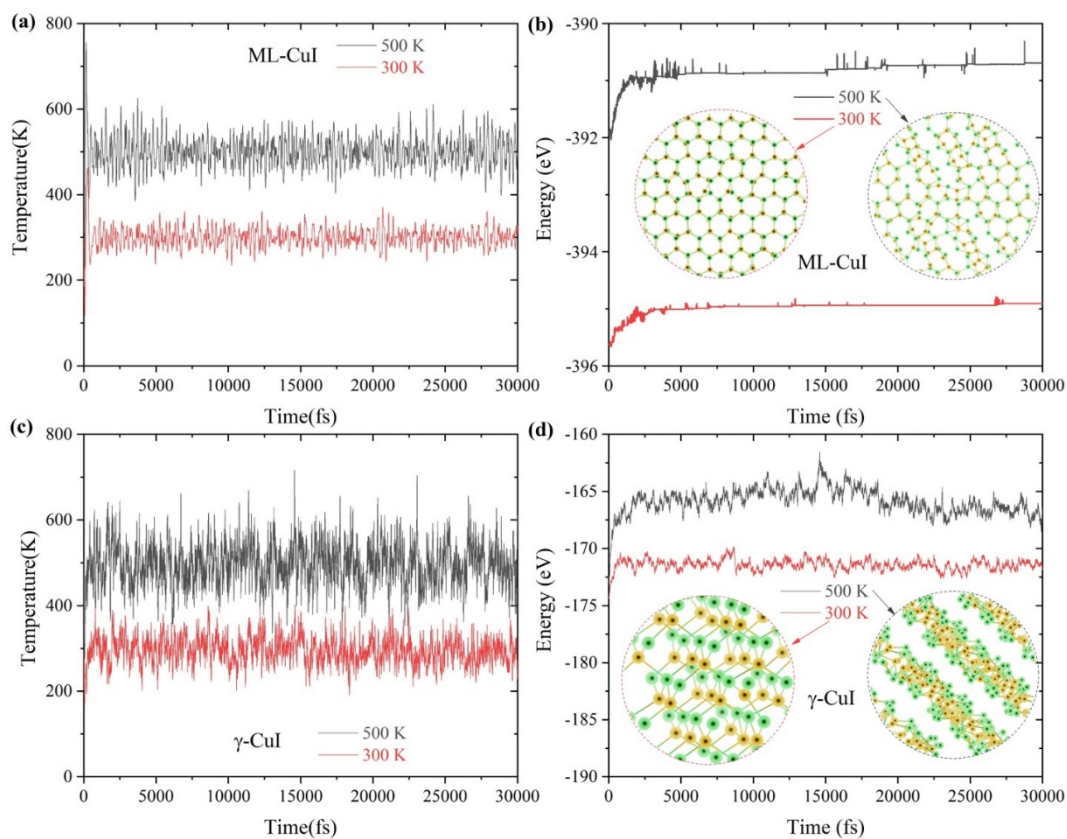


Figure. S1. AIMD simulations at 300 and 500 K for (a-b) monolayer CuI and (c-d) γ -CuI.

Considering that practical applications may contain operating conditions with different temperatures, the high temperature stability of monolayer CuI and γ -CuI is evaluated based on AIMD simulation. The AIMD simulation results at representative temperatures (300 and 500 K) are plotted in Figure S1. It is revealed that both the monolayer CuI and γ -CuI have excellent room temperature stability, while high temperatures may cause phase transitions.